Sulfaguanidine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.21e-02 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.29e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

Image not found
Sulfaguanidine
Measured: 1.03e-02
Predicted: 4.21e-02

Image not found
Azidamfenicol [INN:BAN:DCF]
Measured: 6.77e-02
Predicted: 4.38e-02

Image not found
Arginine
Measured: 1.04
Predicted: 7.61e-01

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Hydrazinecarboximidamide, N-nitro-
Measured: 2.26e-02
Predicted: 2.86e-02